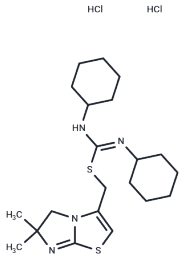
Data Sheet (Cat.No.T11693L)

TargetMol

IT1t dihydrochloride

Chemical Properties



CAS No. : 1092776-63-0

Formula: C21H36Cl2N4S2

Molecular Weight: 479.57

Storage: Powder: -20°C for 3 years | In solvent: -80°C for 1 year
Actual storage temperature shall be subject to the COA.

Biological Description

Description	IT1t dihydrochloride inhibits CXCL12/CXCR4 interaction with IC50 of 2.1 nM. IT1t dihydrochloride is an antagonist of CXCR4.
Targets(IC50)	HIV Protease,CXCR
In vitro	AMD11070 shows antagonistic activity as it dose-dependently inhibits the CXCL12-induced intracellular calcium flux This calcium flux is inhibited by IT1t dihydrochloride with an IC50 of 23.1[1].
In vivo	IT1t dihydrochloride reduces the formation of early metastases of TNBC in a zebrafish xenograft model. After CXCR4 silencing, tumor cell invasion at metastatic sites was effectively reduced [3].

Solubility Information

Solubility	DMSO: 27 mg/mL (56.3 mM),Sonication is recommended. (< 1 mg/ml refers to the product slightly soluble or insoluble)
In vivo Formulation	10% DMSO+40% PEG300+5% Tween 80+45% Saline: 1 mg/mL (2.09 mM),Sonication is recommended. *Please add the solvents sequentially, clarifying the solution as much as possible before adding the next one. Dissolve by heating and/or sonication if necessary. Working solution is recommended to be prepared and used immediately. The formulation provided above is for reference purposes only. In vivo formulations may vary and should be modified based on specific experimental conditions.*

Preparing Stock Solutions

	1mg	5mg	10mg
1 mM	2.0852 mL	10.426 mL	20.852 mL
5 mM	0.417 mL	2.0852 mL	4.1704 mL
10 mM	0.2085 mL	1.0426 mL	2.0852 mL
50 mM	0.0417 mL	0.2085 mL	0.417 mL

Please select the appropriate solvent to prepare the stock solution, according to the solubility of the product in different solvents. Please use it as soon as possible.

Note: The dilution table applies only to solid products. For liquid products, please calculate the stock solution based on the stated concentration and/or density.

Reference

Van Hout A, et al. Comparison of cell-based assays for the identification and evaluation of competitive CXCR4 inhibitors. PLoS One. 2017 Apr 14;12(4):e0176057.
Wu B, et al. Structures of the CXCR4 chemokine GPCR with small-molecule and cyclic peptide antagonists. Science. 2010 Nov 19;330(6007):1066-71.
Tulotta C, et al. Inhibition of signaling between human CXCR4 and zebrafish ligands by the small molecule IT1timpairs the formation of triple-negative breast cancer early metastases in a zebrafish xenograft model. Dis Model Mech. 2016 Feb;9(2):141-53.